Clustering in Machine Learning

Discovering Hidden Patterns in Data

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What is Clustering?

Definition

Clustering is an *unsupervised* machine learning technique that groups similar data points together without prior labeling.

Key Insight: Like organizing books in a library by topic without instructions.

- No labeled examples required
- Discovers hidden structure in raw data
- Most real-world data is unlabeled

Applications:

- Customer segmentation
- Document organization
- Anomaly detection
- Gene clustering

Hard vs Soft Clustering

Hard Clustering

- Each point belongs to *exactly one* cluster
- Binary assignment: 0 or 1
- Example: K-Means

$$x_i \in C_j \text{ for exactly one } j$$

Soft Clustering

- Points have *probability* of membership
- Probabilistic: 0 to 1
- Example: Gaussian Mixture Models

$$\sum_{j=1}^{K} p_{ij} = 1$$

Distance Metrics

Euclidean Distance (Most Common)

$$d(\mathrm{x}, \mathrm{y}) = \sqrt{\sum_{i=1}^{d} (x_i - y_i)^2}$$

Manhattan Distance

$$d(\mathrm{x}, \mathrm{y}) = \sum_{i=1}^{d} |x_i - y_i|$$

Cosine Similarity (Text Data)

$$\text{similarity}(\mathrm{x}, \mathrm{y}) = \frac{\mathrm{x}^T \mathrm{y}}{\|\mathrm{x}\| \|\mathrm{y}\|}$$

K-Means: The Algorithm

1. **Initialize:** Randomly select K points as initial centroids
2. **Assignment:** Assign each point to the nearest centroid

$$C_k = \{\mathrm{x}_i : \|\mathrm{x}_i - \boldsymbol{\mu}_k\| \text{ is minimum}\}$$

3. **Update:** Recalculate centroids

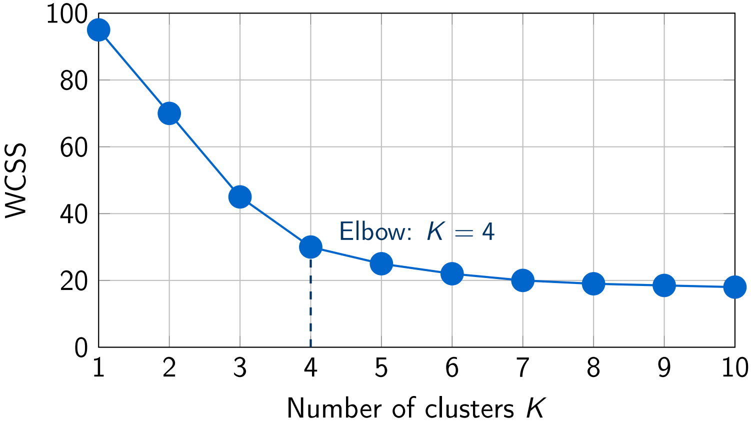
$$\boldsymbol{\mu}_k = \frac{1}{|C_k|} \sum_{\mathrm{x}_i \in C_k} \mathrm{x}_i$$

4. **Repeat:** Steps 2–3 until convergence

Objective: Minimize within-cluster sum of squares (WCSS)

$$\min \sum_{k=1}^{K} \sum_{\mathrm{x}_i \in C_k} \|\mathrm{x}_i - \boldsymbol{\mu}_k\|^2$$

Choosing K: The Elbow Method



Rule: Look for the "elbow" where WCSS levels off.

K-Means: Pros and Cons

Advantages

- Simple and intuitive
- Fast: $O(nKdi)$
- Scales to large data
- Works well with spheres

Limitations

- Must specify K
- Sensitive to initialization
- Assumes spherical clusters
- Sensitive to outliers

Hierarchical Clustering: Bottom-Up

Agglomerative Approach:

1. Start: Each point is its own cluster
2. Find two closest clusters
3. Merge them
4. Repeat until one cluster remains

Result: A dendrogram (tree) showing hierarchical structure

Advantages:

- No need to specify K beforehand
- Produces hierarchy (exploratory)
- Deterministic

Limitations:

- Expensive: $O(n^2 \log n)$ or $O(n^3)$
- Greedy (irreversible merges)

Linkage Criteria

How to measure distance between clusters?

Single Linkage : Minimum distance between clusters

$$d(C_i, C_j) = \min_{x \in C_i, y \in C_j} d(x, y)$$

Complete Linkage : Maximum distance between clusters

$$d(C_i, C_j) = \max_{x \in C_i, y \in C_j} d(x, y)$$

Average Linkage : Average distance between all pairs

$$d(C_i, C_j) = \frac{1}{|C_i||C_j|} \sum_{x \in C_i, y \in C_j} d(x, y)$$

DBSCAN: Density-Based Clustering

Key Idea

Clusters are dense regions separated by sparse regions. Natural identification of noise/outliers.

Parameters:

- ϵ: Radius defining neighborhood
- MinPts: Minimum points to form dense region

Point Types:

- **Core point**: $\geq$ MinPts within ϵ
- **Border point**: Within ϵ of core but not core
- **Noise point**: Neither core nor border

DBSCAN: Pros and Cons

Advantages

- Arbitrary shapes
- Detects outliers
- No need for K
- Robust to noise

Limitations

- Sensitive to ϵ, MinPts
- Varying density issues
- High-dim challenges
- Non-deterministic

Gaussian Mixture Models (GMM)

Probabilistic Model

Data is generated from a mixture of K Gaussian distributions:

$$p(\mathrm{x}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathrm{x}|\boldsymbol{\mu}_k, \Sigma_k)$$

Parameters:

- π_k: Mixing weights (probabilities)
- $\boldsymbol{\mu}_k$: Mean of component k
- Σ_k: Covariance of component k

Soft clustering: Each point has probability of belonging to each component.

EM Algorithm for GMM

Expectation-Maximization:

E-step: Calculate responsibility (posterior probability)

$$\gamma_{ik} = \frac{\pi_k \mathcal{N}(\mathrm{x}_i | \boldsymbol{\mu}_k, \Sigma_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathrm{x}_i | \boldsymbol{\mu}_j, \Sigma_j)}$$

M-step: Update parameters

$$N_k = \sum_{i=1}^{n} \gamma_{ik}$$

$$\boldsymbol{\mu}_k = \frac{1}{N_k} \sum_{i=1}^{n} \gamma_{ik} \mathrm{x}_i$$

$$\pi_k = \frac{N_k}{n}$$

Repeat E and M steps until convergence.

GMM: Pros and Cons

Advantages

- Soft clustering
- Flexible shapes
- Statistical foundation
- Probabilistic

Limitations

- Must specify K
- Sensitive to init.
- Computationally expensive
- Gaussian assumption

Silhouette Score

Definition

For each point i:

$$s(i) = \frac{b(i) - a(i)}{\max\{a(i), b(i)\}}$$

Interpretation:

- $a(i)$: Average distance to points in same cluster
- $b(i)$: Average distance to points in nearest cluster
- Range: $[-1, 1]$
- Higher is better (≈ 1 is excellent)

Use case: Good for evaluating any clustering algorithm

Other Evaluation Metrics

Davies-Bouldin Index

$$DB = \frac{1}{K} \sum_{i=1}^{K} \max_{j \neq i} \left(\frac{\sigma_i + \sigma_j}{d(\boldsymbol{\mu}_i, \boldsymbol{\mu}_j)} \right)$$

Lower is better. Measures average similarity.

Calinski-Harabasz Index

$$CH = \frac{SS_B/(K-1)}{SS_W/(n-K)}$$

Higher is better. Ratio of between/within variance.

Note: These are *internal* metrics (no ground truth needed).

Clustering Algorithms at a Glance

Algorithm	Shape	Scalability	Need K?	Noise Handle
K-Means	Spherical	Excellent	Yes	Poor
Hierarchical	Flexible	Poor	No	Poor
DBSCAN	Arbitrary	Good	No	Excellent
GMM	Ellipsoid	Moderate	Yes	Moderate

Quick Decision Guide:

- Spherical, known K: K-Means
- Hierarchy needed: Hierarchical
- Arbitrary shapes, noisy: DBSCAN
- Soft membership: GMM

Real-World Applications

- **Customer Segmentation**: Purchase behavior, demographics → marketing
- **Image Segmentation**: Pixel clustering by color/texture for computer vision
- **Document Clustering**: News/papers by topic using text features
- **Anomaly Detection**: Points not fitting clusters → fraud, intrusions
- **Recommendation Systems**: Cluster users/items to find similar groups
- **Gene Clustering**: Biology research to understand genetic relationships

Data Preprocessing

Essential Steps:

1. **Feature Scaling**: Standardize to mean 0, variance 1

$$x_i' = \frac{x_i - \mu}{\sigma}$$

   Without this, large-range features dominate distance!

2. **Dimensionality Reduction**: Use PCA/t-SNE for high-dimensional data (curse of dimensionality)

3. **Handle Missing Values**: Impute or remove before clustering

Workflow: Best Practices

1. **Explore Data**: Visualize, understand features
2. **Preprocess**: Scale, handle outliers, reduce dimensions
3. **Try Multiple Algorithms**: Start simple (K-Means), then explore others
4. **Evaluate**: Use silhouette score, Davies-Bouldin, etc.
5. **Validate with Domain Knowledge**: Does the clustering make sense?
6. **Iterate**: Refine based on results

Remember: Often no single "correct" answer—different clusterings reveal different aspects!

Key Takeaways

- **Clustering** discovers structure in unlabeled data
- **Four main approaches**:
  - K-Means: Fast for spherical clusters
  - Hierarchical: Exploratory with dendrograms
  - DBSCAN: Handles arbitrary shapes and noise
  - GMM: Probabilistic with soft assignments
- **No single best algorithm**—choose based on your data and goals
- **Preprocessing matters**: Scale features, handle high dimensions
- **Evaluation is critical**: Use multiple internal metrics

Thank You!

Questions?

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